Detailed Balance

The final principal governing ionized regions is detailed balance. In a steady state, the fraction of ions with electrons in any state will remain constant with time. In other words, for an ensemble of atoms of species X, the number of electrons entering a given level, *i*, will equal the number of electrons leaving that level.

For example, if one models an atom with hundreds (or thousands) of energy levels, a separate equation can be written down for each level.

$$N_e N_X \alpha_i(T_e) + \sum_{j>i} N_j A_{j,i} + \sum_{j\neq i} N_e N_j q_{j,i} = \sum_{j<i} N_i A_{i,j} + \sum_{j\neq i} N_e N_i q_{i,j}$$

Detailed Balance

$$N_e N_X \alpha_i(T_e) + \sum_{j>i} N_j A_{j,i} + \sum_{j\neq i} N_e N_j q_{j,i} = \sum_{j<i} N_i A_{i,j} + \sum_{j\neq i} N_e N_i q_{i,j}$$

This equation is for level *i*. Note the terms:

- The unknowns in the equation are the number density of atoms with electrons in levels 1, 2, 3 … *N*. In other words, N_1, N_2, N_3, etc.
- The first term represents recombinations directly into level *i*. It depends on the recombination coefficient to that level, $\alpha_i(T_e)$, the density of the free electrons, N_e, and the ion's abundance, $N_X = \sum N_i$.
- The 2nd and 4th terms are radiative decays from upper levels into level *i* and from level *i* into lower levels. These only depend on the Einstein A coefficients, which are known from atomic physics.
- The 3rd and 5th terms are collisions from all levels into level *i*, and from *i* into all other levels. These depend on the temperature and density of the free electrons, and the quantum mechanical collision strengths, which are (sort of) known from atomic physics.

Detailed Balance

$$N_e N_X \alpha_i(T_e) + \sum_{j>i} N_j A_{j,i} + \sum_{j \neq i} N_e N_j q_{j,i} = \sum_{j<i} N_i A_{i,j} + \sum_{j \neq i} N_e N_i q_{i,j}$$

In other words, for a given value for the density and temperature of the free electrons, the only unknowns in the detailed balance equation are the number density of ions in each level, N_i. If one models an atom with 100 levels, that means there are 100 (linear) equations and 100 unknowns. This is what linear algebra is made for.

In case you're wondering, the equation of detailed balance neglects absorptions. This is generally a good assumption for all levels except possibly the ground state. (Recall that in the ISM, almost all the atoms are in the ground state.) But, as you'll see, there is a way to handle this. (It also neglects stimulated emission, which is fine.)

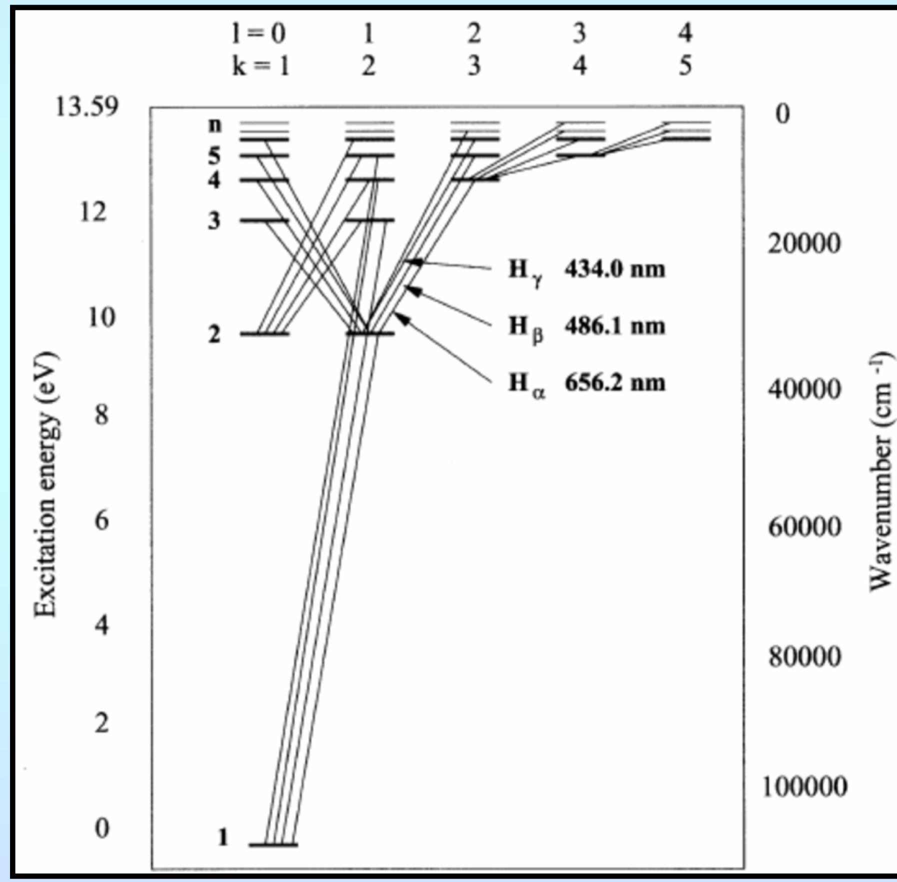
Note that there is one additional equation in detailed balance. The total abundance of species X is

$$\sum_i^n N_i = N_X$$

Hydrogen and Detailed Balance

$$N_e N_X \alpha_i(T_e) + \sum_{j>i} N_j A_{j,i} + \cancel{\sum_{j\neq i} N_e N_j q_{j,i}} = \sum_{j<i} N_i A_{i,j} + \cancel{\sum_{j\neq i} N_e N_i q_{i,j}}$$

For hydrogen, the energy difference between the ground and first state is too large for collisional excitation. Also (almost) every excited level has a permitted transition to a lower level ($A \gtrsim 10^5$ sec^{-1}), so the electrons don't stay excited long enough to be collided out. (What's the exception?)



So the collisional terms in the detailed balance equation can be neglected.

Hydrogen and Detailed Balance

$$N_e N_X \alpha_i(T_e) + \sum_{j>i} N_j A_{j,i} = \sum_{j<i} N_i A_{i,j}$$

There are a number of interesting facets to the detailed balance equation for hydrogen.

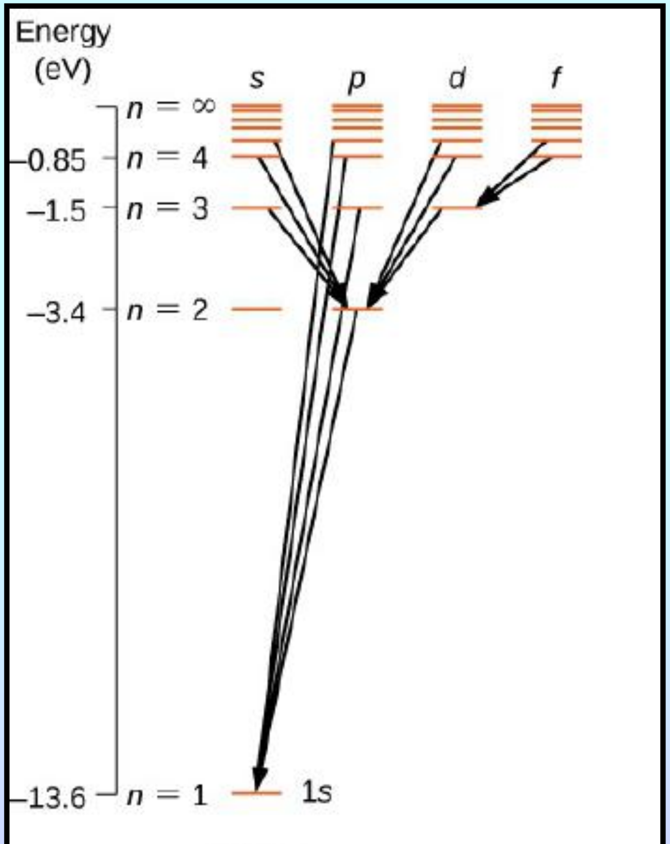
- The absorption cross-sections to Lyman series photons are much greater that those for ionizing photons. (The cross-section for Lyα absorption is ~ 10,000 larger than for a 912 Å photon which causes ionization.) So one can make the equivalent of the "on-the-spot" approximation and say that all transitions to the ground state create photons that are immediately re-absorbed. In other words, transitions to the ground state effectively do not exist. This is called **Case B**; most objects in the universe are in the Case B regime.

Hydrogen and Detailed Balance

$$N_e N_X \alpha_i(T_e) + \sum_{j>i} N_j A_{j,i} = \sum_{j<i} N_i A_{i,j}$$

There are a number of interesting facets to the detailed balance equation for hydrogen.

- If transitions to the ground state do not exist, then all recombinations must eventually go to *n*=2. That means a Balmer line photon. In other words: every ionization is followed by a recombination, and every recombination creates a Balmer line photon. Count the Balmer line photons, and you count the number of ionizing photons.



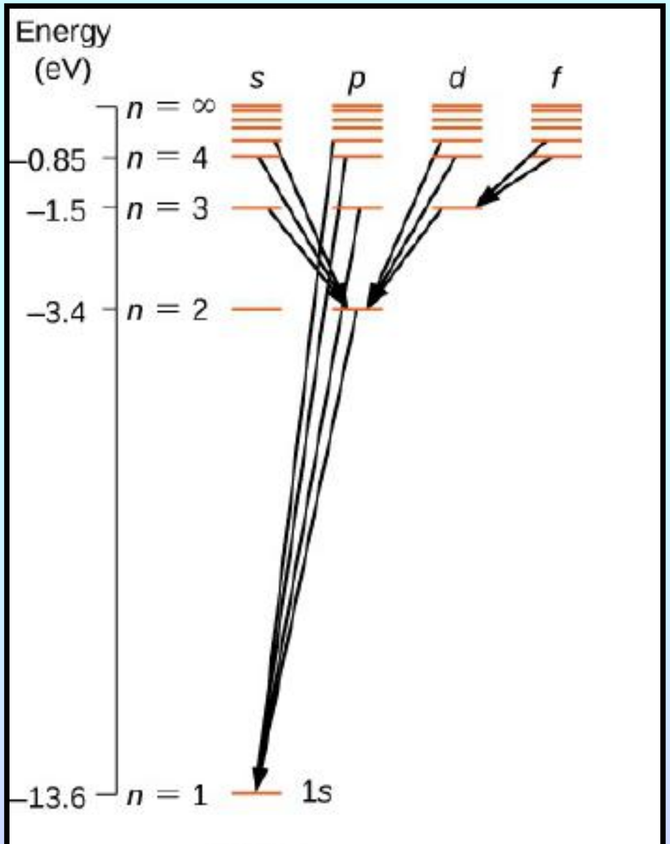
(a) Hydrogen

Hydrogen and Detailed Balance

$$N_e N_X \alpha_i(T_e) + \sum_{j>i} N_j A_{j,i} = \sum_{j<i} N_i A_{i,j}$$

There are a number of interesting facets to the detailed balance equation for hydrogen.

- There $(2L+1)=3$ states associated with the p orbital, but only 1 with the s orbital. So ~75% of decaying electrons wind up in the n=2 p-state. (Actually, detailed calculations of the cascading electrons give a value of 68%.)



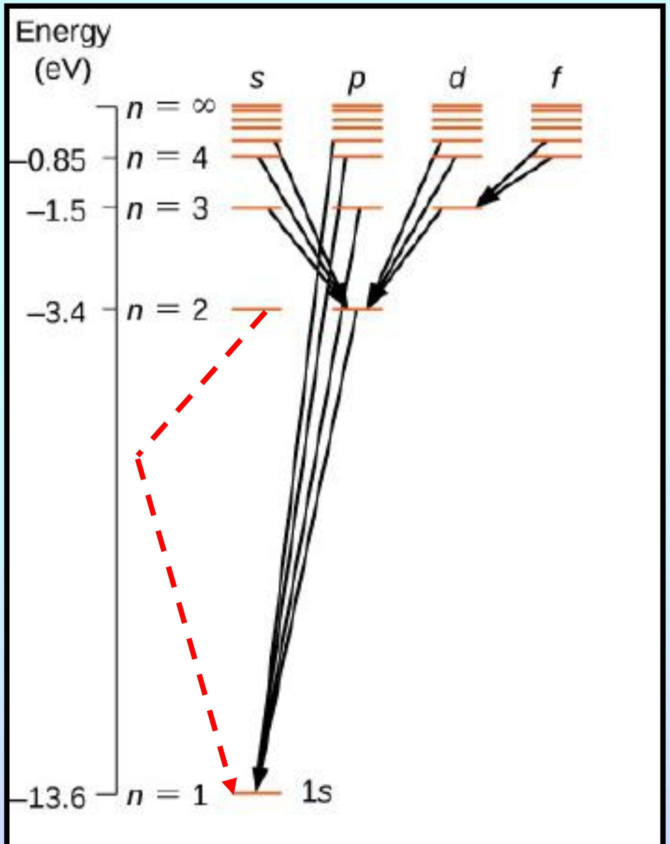
(a) Hydrogen

Hydrogen and Detailed Balance

$$N_e N_X \alpha_i(T_e) + \sum_{j>i} N_j A_{j,i} = \sum_{j<i} N_i A_{i,j}$$

There are a number of interesting facets to the detailed balance equation for hydrogen.

- What happens when the electrons reach n=2? If the electron is in the s orbital (L=0), there's no way down to the ground state (L=0) through simple physics. It must either be collided out or decay via a forbidden relativistic process that causes two photons to be emitted (A = 8.23 sec^{-1}). The two photons add up to 10.2 eV, but the division of energies is probabilistic.



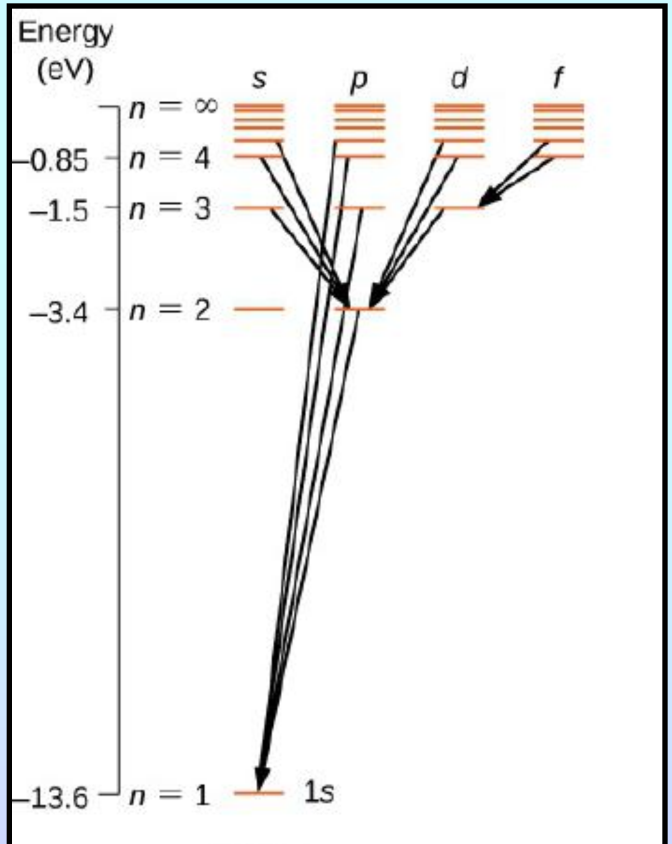
(a) Hydrogen

Hydrogen and Detailed Balance

$$N_e N_X \alpha_i(T_e) + \sum_{j>i} N_j A_{j,i} = \sum_{j<i} N_i A_{i,j}$$

There are a number of interesting facets to the detailed balance equation for hydrogen.

- If the electron is in the p orbital (L=1), then the electron decays almost immediately ($A = 6.26 \times 10^8$ sec^{-1}) by emitting Lyα. Since the cross-section for absorption is huge, this photon is quickly absorbed, then re-emitted, then re-absorbed, etc. The photon bounces around, until it either escapes via velocity shifts, or is destroyed when it runs into a particle of dust.



(a) Hydrogen

Hydrogen and Detailed Balance

$$N_e N_X \alpha_i(T_e) + \sum_{j>i} N_j A_{j,i} = \sum_{j<i} N_i A_{i,j}$$

There are a number of interesting facets to the detailed balance equation for hydrogen.

- There are many terms in the detailed balance equation (one for every N_i), but only one term depends on the outside conditions (the recombination rate). Every other term is simply a function of the atomic constants, A_i. As a result, as long as collisions are insignificant, the solution to these equations (the N_i values) depend very little on what's happening in the outside world. That means that the relative line strengths (i.e., $N_i\ A_{i,j} \cdot h\ \nu_{i,j}$) do not change much at all! If you know one line, you know them all!

Hydrogen (Case B) Line Ratios

Temperature	10,000			20,000		
Density (cm^{-3})	10^2	10^4	10^6	10^2	10^4	10^6
Hα/Hβ	2.859	2.847	2.807	2.744	2.740	2.724
Hγ/Hβ	0.468	0.469	0.471	0.475	0.476	0.476
Hδ/Hβ	0.259	0.260	0.262	0.264	0.264	0.266
Hε/Hβ	0.159	0.159	0.163	0.163	0.163	0.164
Hζ/Hβ	0.105	0.105	0.110	0.107	0.107	0.110
Paα/Hβ	0.338	0.332	0.317	0.284	0.281	0.280
Paβ/Hβ	0.348	0.345	0.335	0.305	0.304	0.300

Ionized gas regions almost always have electron temperatures between ~8,000 and ~14,000. (You'll eventually see why.) As you can see, the hydrogen (and helium) recombination line ratios depend very little on the external conditions.

If one observes Hα/Hβ > 3, it is almost always due to reddening.

Hydrogen (Case B) Line Ratios

Temperature	**10,000**			**20,000**		
Density (cm^{-3})	10^2	10^4	10^6	10^2	10^4	10^6
Hα/Hβ	2.859	2.847	2.807	2.744	2.740	2.724
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Paα/Hβ	0.338	0.332	0.317	0.284	0.281	0.280
Paβ/Hβ	0.348	0.345	0.335	0.305	0.304	0.300
$\alpha_{H\beta}$(eff) (cm^3/s)	3.02×10^{-14}			1.61×10^{-14}		

This also means that one can use the total recombination coefficient, α_B, to compute a coefficient for recombinations that eventually create a specific line, say, Hβ. In other words, in addition to *relative* line ratios, you also have the total Hβ emission, with $\varepsilon(H\beta) = N_e \, N_p \, \alpha_{H\beta}(\mathrm{eff}) \cdot h \, \nu_{H\beta}$ ergs/cm^3/s.

Hydrogen (Case B) Line Ratios

Temperature	**10,000**			**20,000**		
Density (cm^{-3})	10^2	10^4	10^6	10^2	10^4	10^6
$H\alpha/H\beta$	2.859	2.847	2.807	2.744	2.740	2.724
$H\gamma/H\beta$	0.468	0.469	0.471	0.475	0.476	0.476
$H\delta/H\beta$	0.259	0.260	0.262	0.264	0.264	0.266
$H\varepsilon/H\beta$	0.159	0.159	0.163	0.163	0.163	0.164
$H\zeta/H\beta$	0.105	0.105	0.110	0.107	0.107	0.110
$Pa\alpha/H\beta$	0.338	0.332	0.317	0.284	0.281	0.280
$Pa\beta/H\beta$	0.348	0.345	0.335	0.305	0.304	0.300
$\alpha_{H\beta}$(eff) (cm^3/s)	3.02×10^{-14}			1.61×10^{-14}		

This same recombination-line physics that applies to the hydrogen also applies to helium and He^+. There are effective recombination rates for He I λ5876 and He II λ4686, the He line-ratios are fixed, and the equation for the radii of the helium Strömgren spheres are the same.

Reddening Diagnostic

Recall that, in magnitudes, the extinction at any wavelength is

$$A_\lambda = R_\lambda\, E(B\text{-}V)$$

where R_λ is defined by the extinction law. The observed strengths of the Hα and Hβ lines are thus related to their true strengths by

$$f_{\mathrm{H}\alpha}^{\mathrm{obs}} = f_{\mathrm{H}\alpha}^{\mathrm{true}}\ 10^{-R_{\mathrm{H}\alpha} E(B-V)/2.5}$$
$$f_{\mathrm{H}\beta}^{\mathrm{obs}} = f_{\mathrm{H}\beta}^{\mathrm{true}}\ 10^{-R_{\mathrm{H}\beta} E(B-V)/2.5}$$

If we divide the two equations, and take the log

$$\log\left(\frac{f_{\mathrm{H}\alpha}}{f_{\mathrm{H}\beta}}\right)_{\mathrm{obs}} = \log\left(\frac{f_{\mathrm{H}\alpha}}{f_{\mathrm{H}\beta}}\right)_{\mathrm{true}} + (R_{\mathrm{H}\beta} - R_{\mathrm{H}\alpha})E(B-V)/2.5$$

For the mean Milky Way extinction law, $R_{\mathrm{H}\alpha}$=2.535 and $R_{\mathrm{H}\beta}$=3.609. Since we observe Hα/Hβ, and the true ratio is 2.86, we can determine $E(B-V)$ and correct all the emission lines via

$$f_\lambda^{\mathrm{true}} = f_\lambda^{\mathrm{obs}} 10^{R_\lambda E(B-V)/2.5}$$

Reddening Diagnostic

Note: one peculiarity of people who study emission-line regions is that they rarely speak in terms of $E(B\text{-}V)$. Instead, they always quote $c_{H\beta}$, which is the logarithmic total extinction at Hβ.

Although that phrase contains a lot of syllables, it really is simple: recall that at any wavelength, the total extinction in magnitudes is

$$A_\lambda = R_\lambda \, E(B\text{-}V)$$

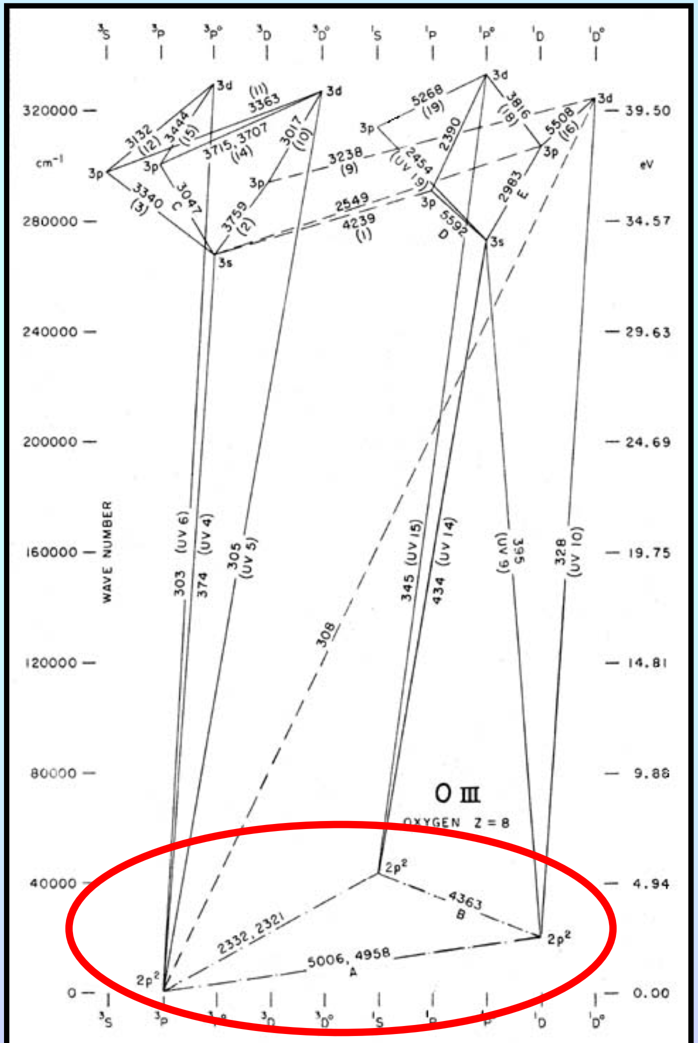
and a magnitude is 2.5 times the log of a quantity. So

$$c_{H\beta} = R_{H\beta} \, E(B\text{-}V) \, / \, 2.5$$

Metals and Detailed Balance

$$\cancel{N_e N_X \alpha_X(T_e)} + \sum_{j>i} N_j A_{j,i} + \sum_{j \neq i} N_e N_j q_{j,i} = \sum_{j<i} N_i A_{i,j} + \sum_{j \neq i} N_e N_i q_{i,j}$$

Elements heavier than helium are rare, so recombinations play an extremely minor role in their detailed balance equation. Moreover, since the transitions between low-lying levels are all forbidden, absorptions do not occur. Detailed balance is therefore all about collisional excitation and radiative decay.

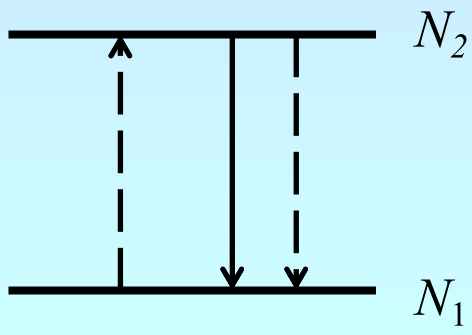


Because of the *large* separations between levels with different n values, for the most important species, one really only has to worry about 5 energy levels! So detailed balance means solving five equations with five unknowns. Easy!

Critical Density

When do we see forbidden lines? Consider a two level atom.

There is only one way into level 2: by collisions up from level 1. But there are two ways out:



- By radiative decays downward, $N_2\,A_{2,1}$
- By collisional de-excitations, $N_2\,N_e\,q_{2,1}$

When the radiative decays take so long that collisions are more likely to occur, the forbidden lines go away, i.e., when the electron density $N_e(\text{crit}) > A_{2,1} / q_{2,1}$. For a multi-level atom, we therefore define the critical density of any level, i, as

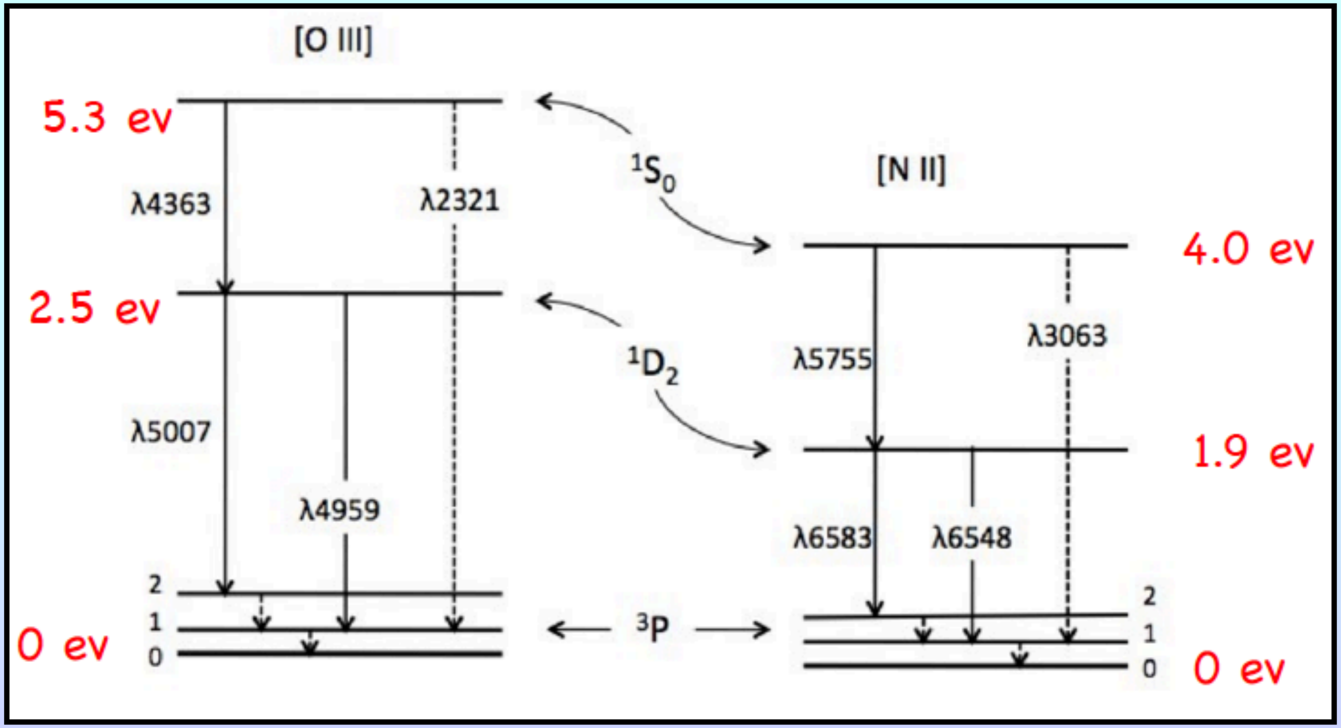
$$N_e(\text{crit}) > \frac{\sum_{j<i} A_{i,j}}{\sum_{j\neq i} q_{i,j}}$$

When the electron density is greater than this, the emission lines go away.

Line Diagnostics

Just as for hydrogen, the relative strengths of collisionally-excited forbidden lines carry a huge amount of information.

- Some ratios are fixed by physics. The λ5007 line of [O III] comes from the exact same level as the [O III] λ4959 line. The ratio of those lines is simply the ratio of the A-values. (The λ5007 line is always 2.98 times that of λ4959.)



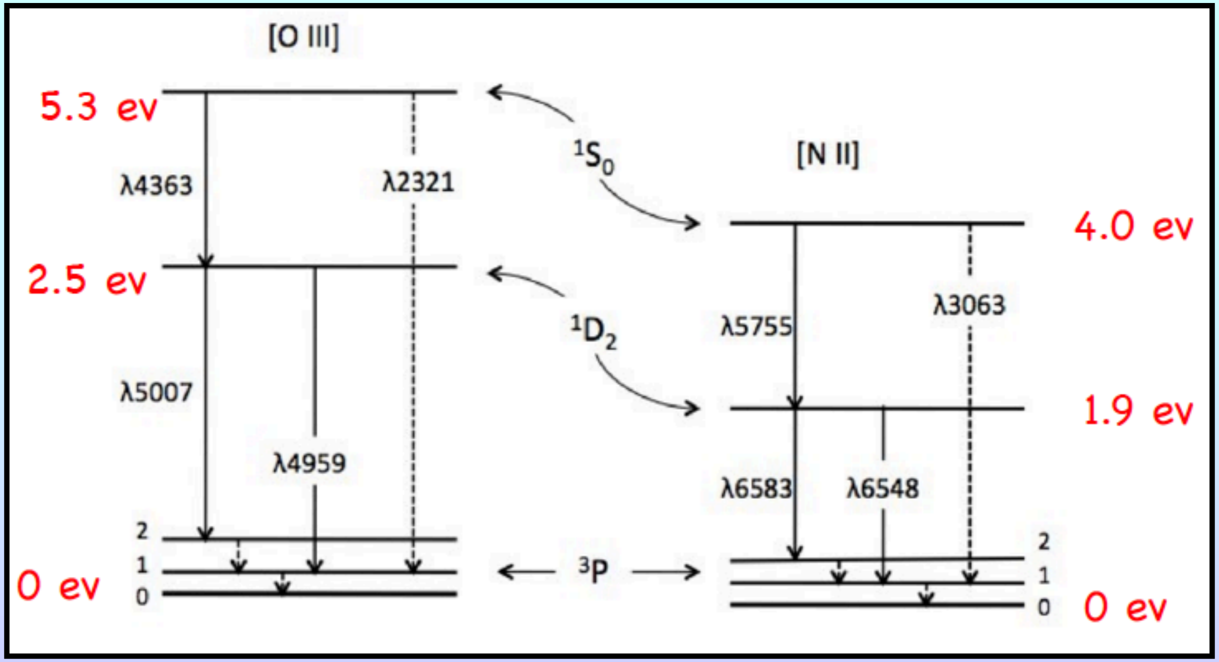
Line Diagnostics

- Ions with 2 or 4 electrons in their p-shell (p^2 or p^4) have their energy levels broken into a 3-1-1 configuration. These are good for measuring electron temperature. Recall that the rate of collisions between any two levels is

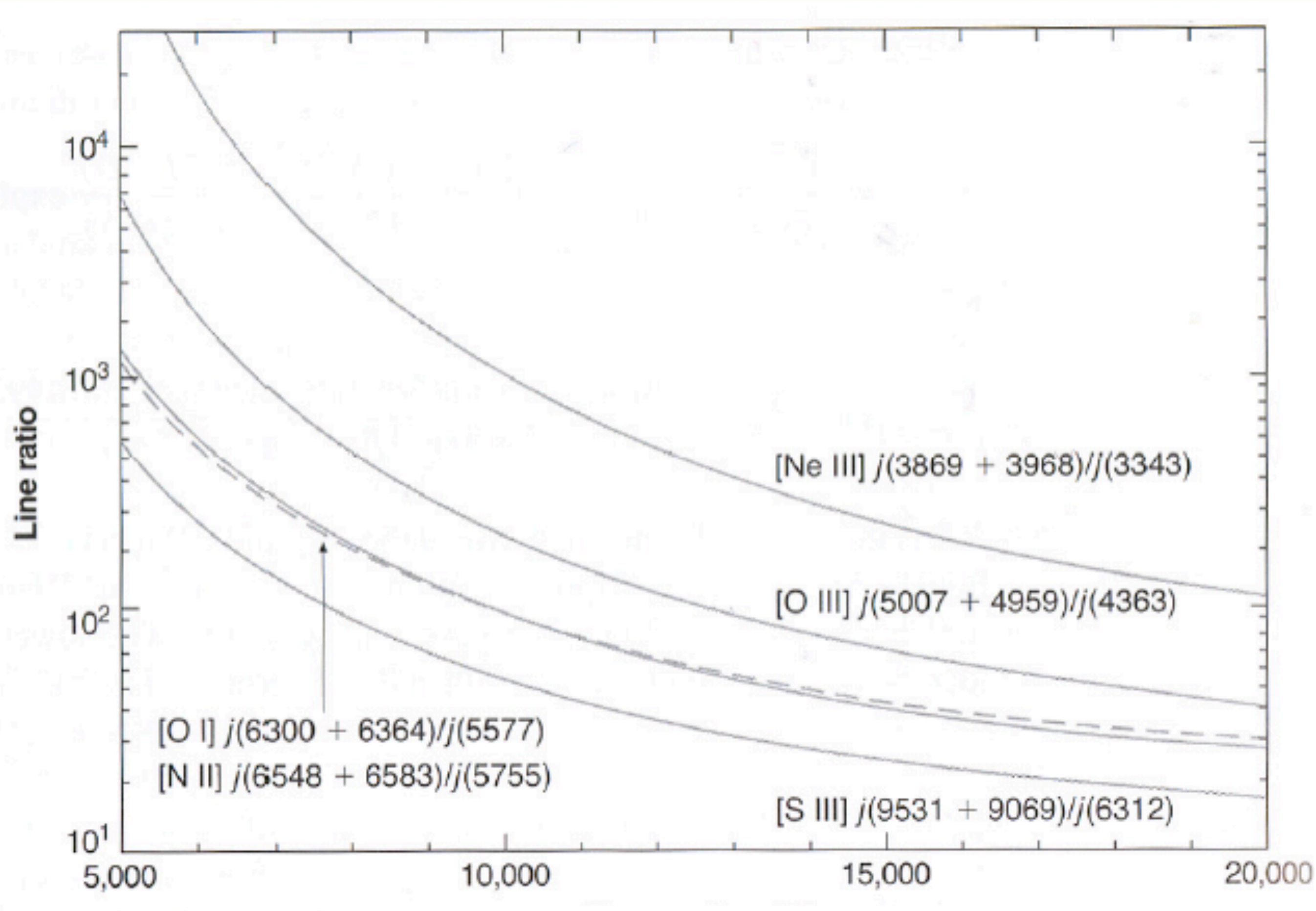
$$q_{i,j} = 8.629 \times 10^{-6} \frac{\Omega_{i,j}}{\omega_i T_e^{1/2}} e^{-\Delta E_{i,j}/kT_e} \text{ cm}^3 \text{ s}^{-1}$$

The exponential factor is important – it is a lot harder to push an electron up to the top level than it is the middle level.

The ratio of a line from an upper level (such as [O III] λ4363) to that from a lower level (i.e., [O III] λ5007) gives a measure of the temperature of the free electrons.



Temperature Diagnostics



Temperature (Low Density Limit)

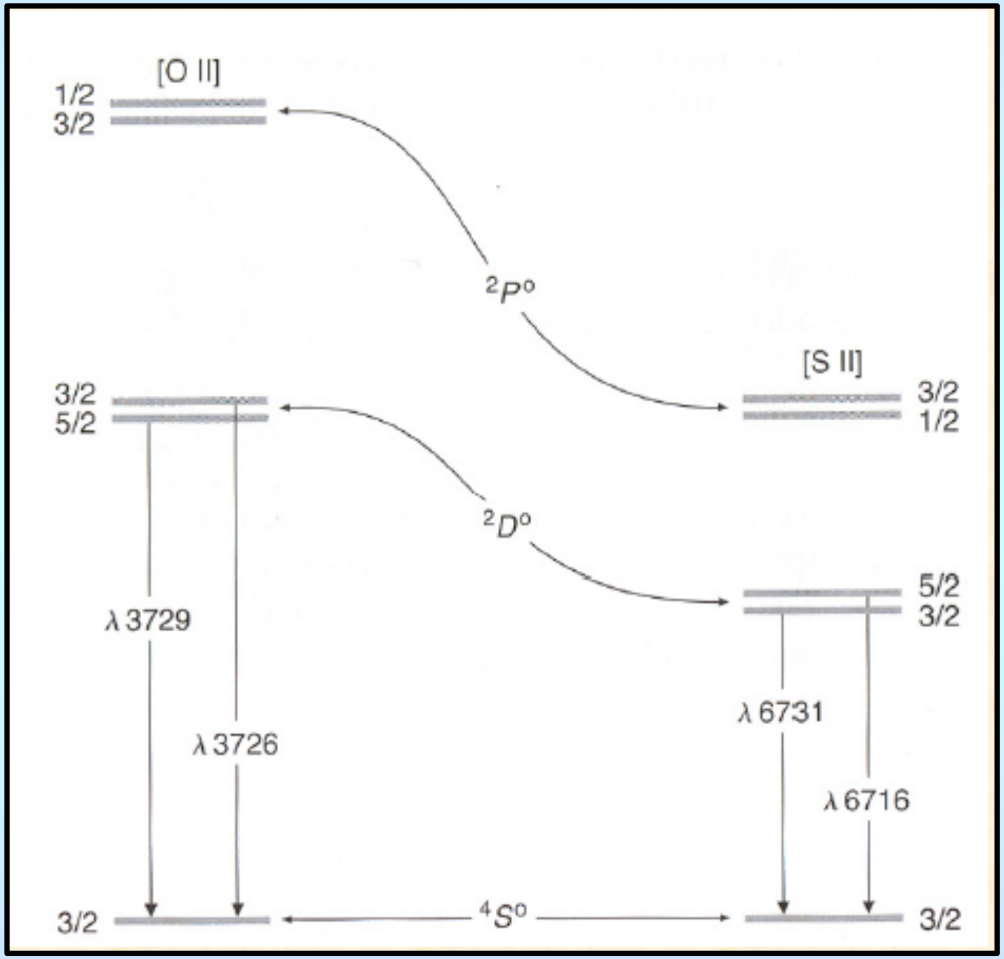
The good news: the line ratios give you an accurate temperature of the free electrons.

The bad news: the upper ("auroral") lines may be *very* weak.

Density Diagnostics

- While p^2 and p^4 ions give the electron temperature, data on the electron density comes from the 2-2-1 structure of the p^3 ions.

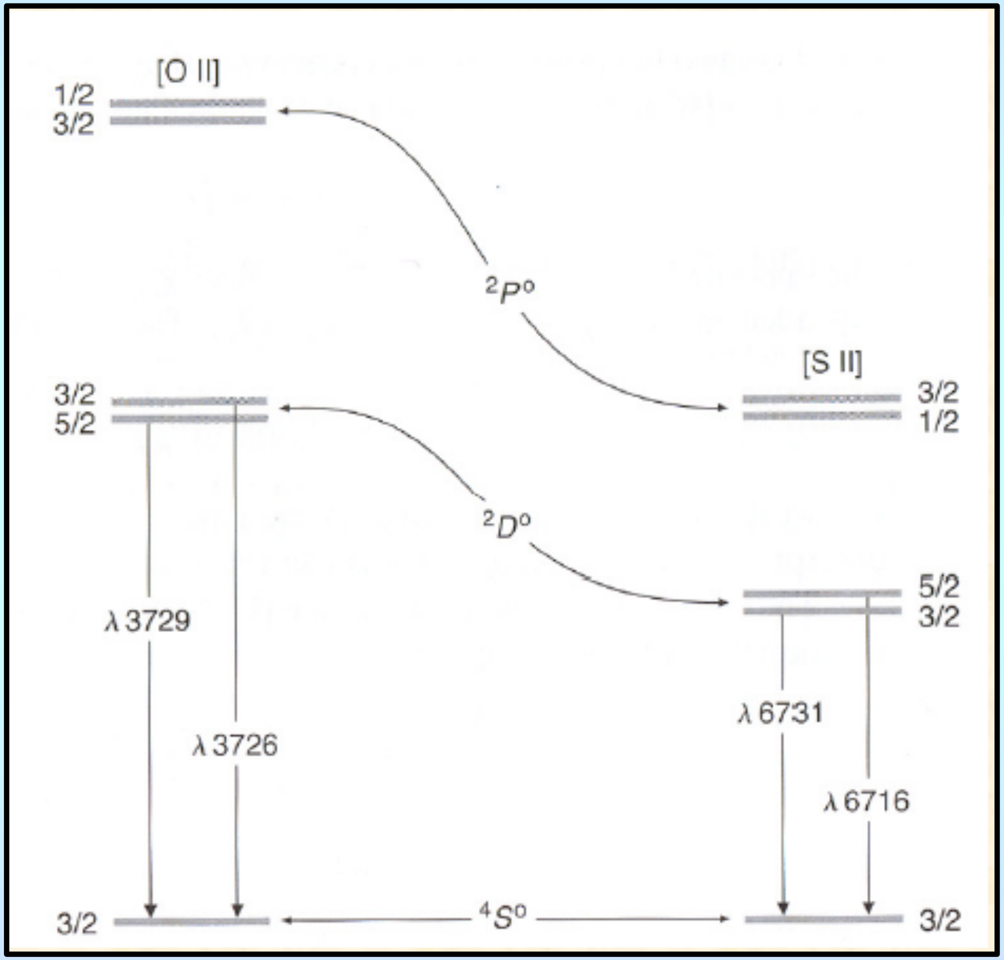
Since the energy difference between the two ^2D levels is negligible, any collision that can reach one can reach the other. So the levels are populated equally. But the statistical weight of $^2D_{5/2}$ is 6, while that of $^2D_{3/2}$ is 4. If every collision up results in a decay down, the λ3729 line will be 1.5 times as strong as λ3726, as there are 1.5 times more electrons in that state.



Density Diagnostics

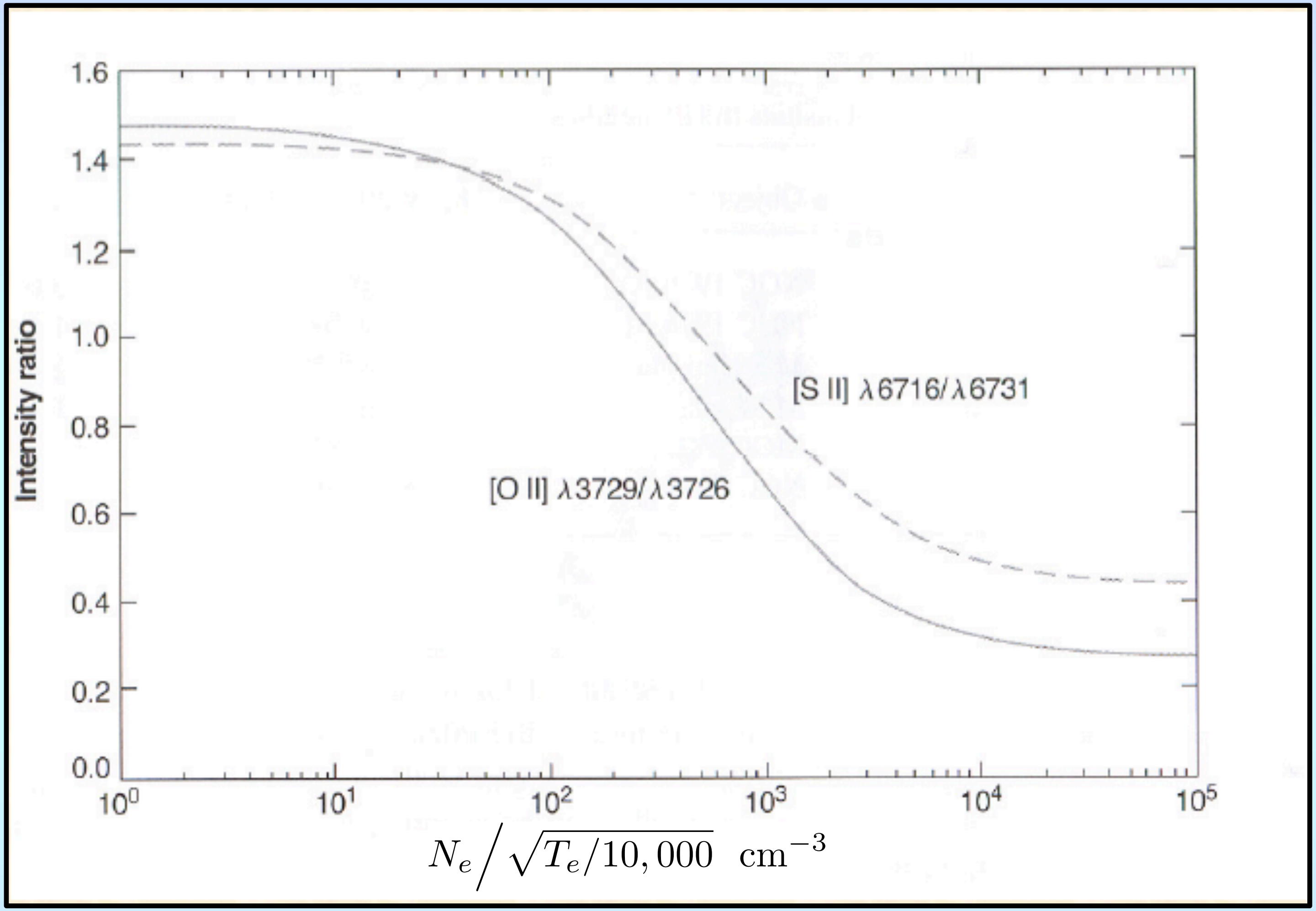
- While p^2 and p^4 ions give the electron temperature, data on the electron density comes from the 2-2-1 structure of the p^3 ions.

On the other hand, if the density is high enough, collisions will occur when the electrons are excited. Electrons will constantly be redistributed between the two states, and, since the A value for the λ3726 line is 5 times greater than that for the λ3727 line, there will be a 5 times greater chance of a decay. So



$$\frac{I(\lambda 3727)}{I(\lambda 3727)} = \frac{\omega_{3729} A_{3729}}{\omega_{3726} A_{3726}} = 1.5\, \frac{A_{3727}}{A_{3726}} = 0.3$$

Density Diagnostics



The good news: the line ratios give you an accurate density.

The bad news: the two oxygen lines are very close together and may be blended. Often times, the lines are just referred to as "3727".

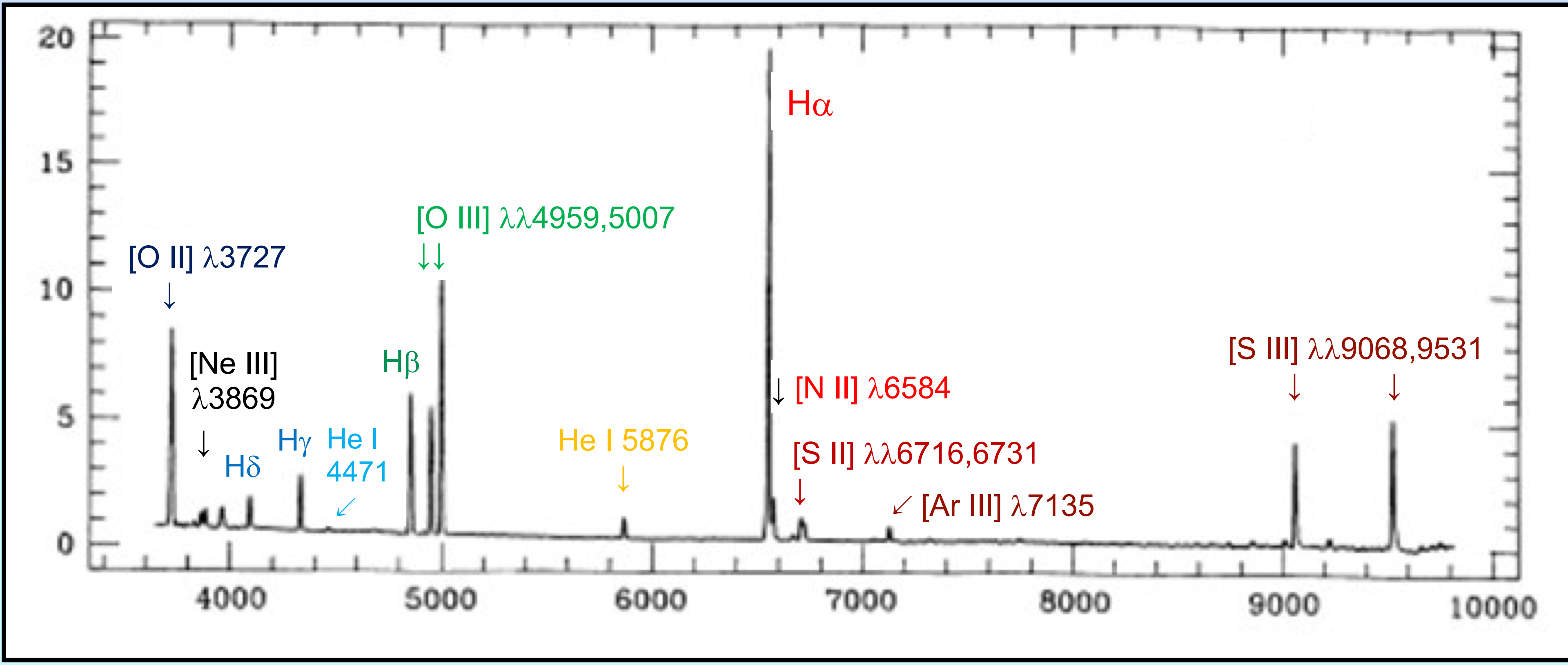
Ionization Parameter

How much of a species is in ionization state i, i+1, i+2, etc. depends on two factors:

- The temperature of the ionizing source. Is the source producing photons capable of taking the 2nd or 3rd electron off a species?
- The ionization parameter, i.e., the ratio of the flux of ionizing photons to the density of electrons, $\Gamma = (Q/4\pi r^2) / N_e c$, where Q is the number of ionizing photons per second being generated by the star, r is the distance from the star, and the speed of light is there just to make the number dimensionless. If the ionization flux is low, it may not matter if there are photons capable of stripping the second electron off a species: the first electron will recombine long before a second ionization occurs.

Usually, one can estimate the ionization parameter by looking at the relative strengths of H, He, and He^+ and combining that information with an estimate of the N_e.

Thought Experiment



How might the line-strengths change if the metallicity were decreased?

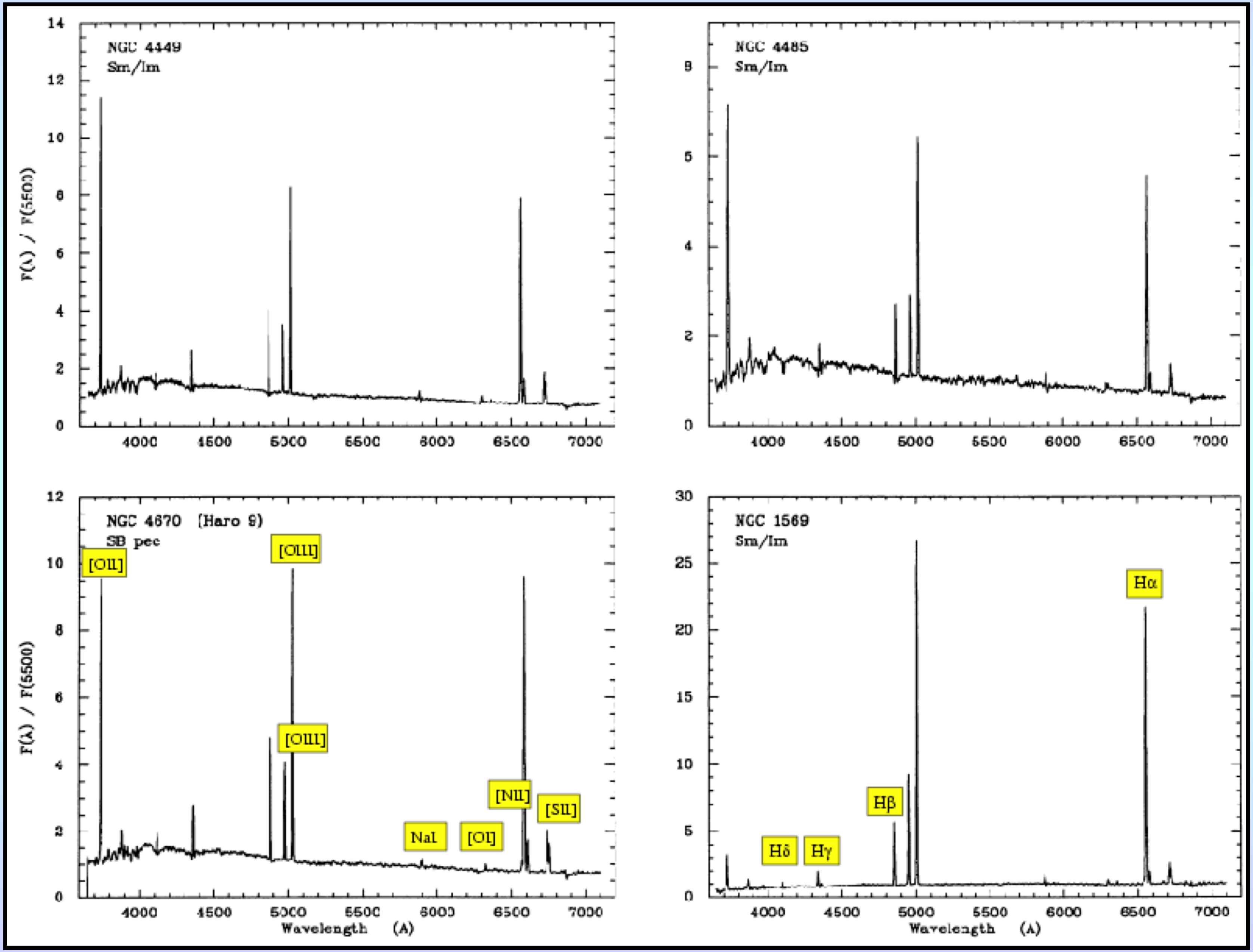
Thought Experiment

If the metallicity were decreased:

- The number of O, Ne, N, S, and Ar atoms would decrease.
- The emission lines from these metals would be weaker.
- Less total energy emitted from the nebula would be less; the nebula's free electrons would be hotter.
- The electrons will be moving faster; the number of collisions per second would increase.
- Each metal ion would undergo more frequent collisional excitation. The rate of emission from each metal ion would increase, and nebular cooling would increase.

The moral: there is a thermostat effect with metals. Fewer metals lead to a hotter nebula, thus more emission per ion and greater cooling per ion. A change in metallicity generally creates hotter nebulae, but whether the line-strengths increase or decrease is complicated.

Emission Line Spectra



Abundance Measurements

The strength of a collisionally excited emission line is given by

$$\epsilon = N_e N_i \, q_{i,j} \cdot h\nu_{i,j} \quad \text{where}$$

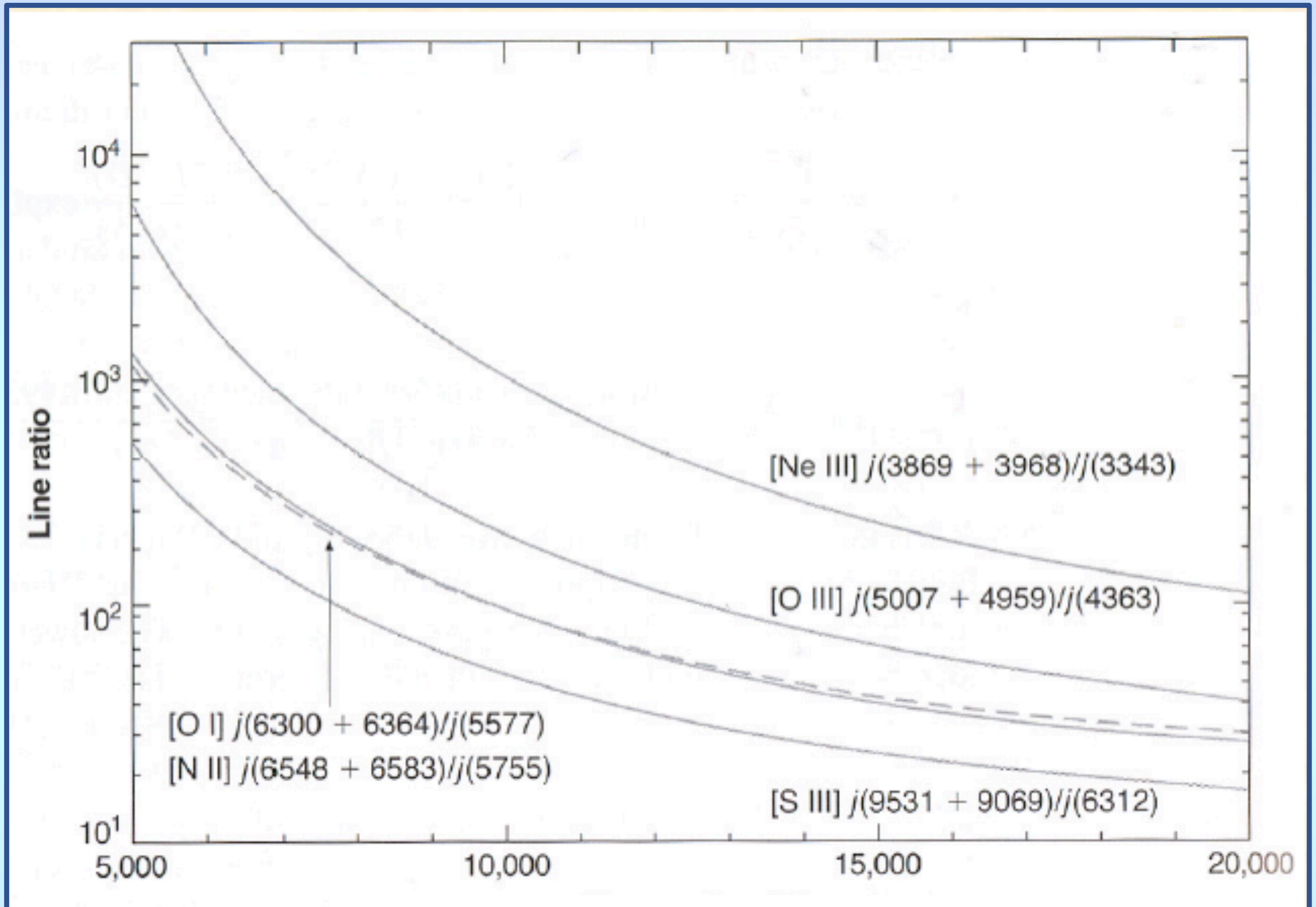
$$q_{i,j} = 8.629 \times 10^{-6} \frac{\Omega_{i,j}}{\omega_i T_e^{1/2}} e^{-\Delta E/kT_e} \text{ cm}^3 \text{ s}^{-1}$$

(For downward collisions, it's the same equation but without the exponential Boltzmann factor.)

Since $\Omega_{i,j}$ and $\omega_{i,j}$ are constants of atomic physics, this means that you can directly measure the abundance of an ion, N_i, *if* you can fix the electron temperature and density of the nebula via the line diagnostics.

Of course, the abundance of a single ion, say, O^{++} is not the same as the abundance of oxygen. Ideally, to measure the oxygen abundance, you need measurements for O^0, O^+, O^{++}, O^{+++}, etc., though one can usually get a good estimate with just 2 states.

Temperature Diagnostics

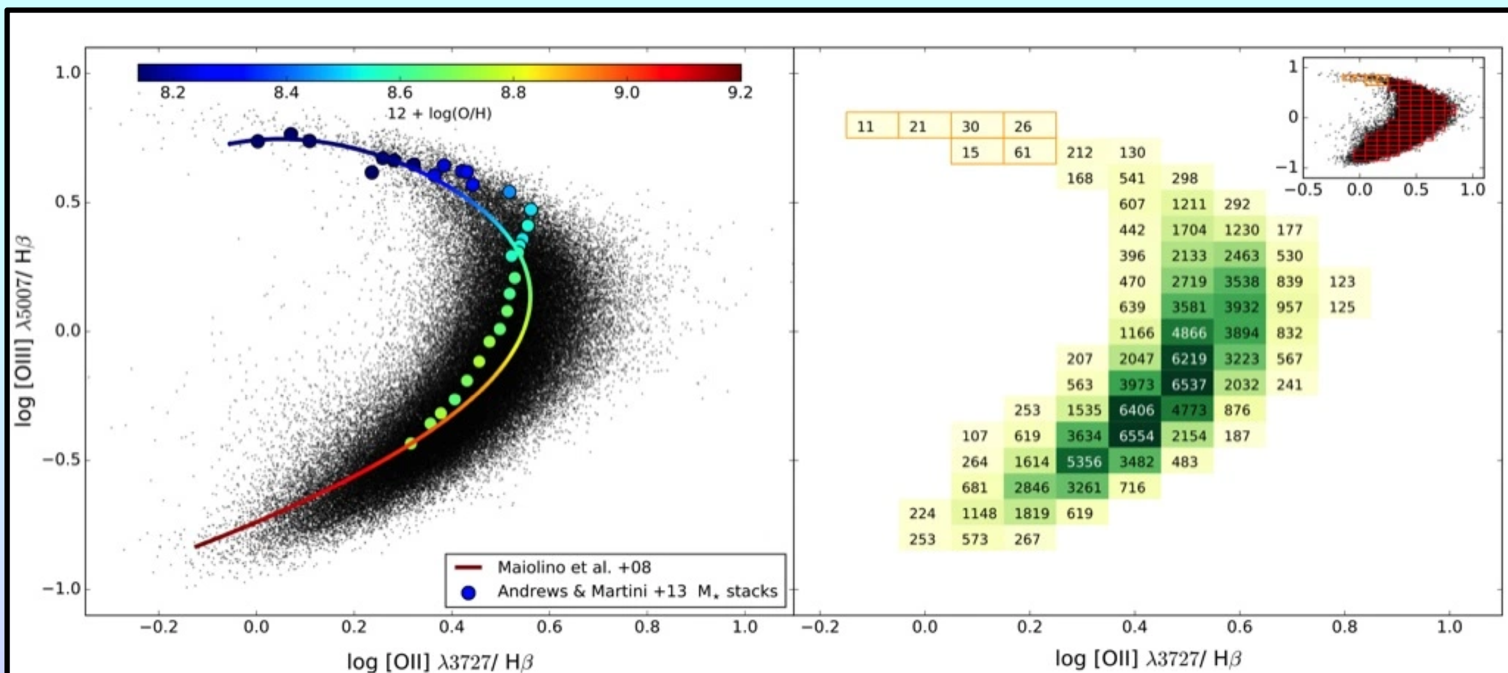


Temperature (Low Density Limit)

But remember: determining the temperature of a nebula often relies on measuring a faint emission line (generally [O III] λ4363). This line can be 50 to 100 times fainter than [O III] λ5007.

Abundance Measurements

If the key emission-line diagnostics for electron temperature (and, to a lesser extent, density) are not available, then it is impossible to obtain a direct measurement of abundance from the emission lines. However, various groups have produced empirical strong-line calibrations using well-observed local objects. The assumption is that distant/fainter sources are identical to the bright systems of the local neighborhood.



Summary of Results

- Most objects are "optically thick" to ionizing photons. As a result, the recombination lines of hydrogen and helium allow you to count the number of photons shortward of their ionization edge and estimate an object's far-UV spectrum. The interpretation of these lines does, however, depend on the density squared.

- The hydrogen (and helium) line ratios are (to a very high degree) fixed by atomic physics, and do not depend on nebular conditions. In particular $H\alpha/H\beta = 2.86$ (with at most a couple percent error). If one measures a higher ratio, it is almost certainly due to interstellar reddening. If one measures a lower ratio, then something is wrong.

- The collisionally excited forbidden lines of O, N, S, Ar, and Ne allow one to measure nebular conditions, i.e., the density and temperature of the free electrons. They also provide information on the "ionization parameter", i.e., the density ratio of ionizing photons to atoms in the ISM, and the abundance of the gas.

Summary of Results

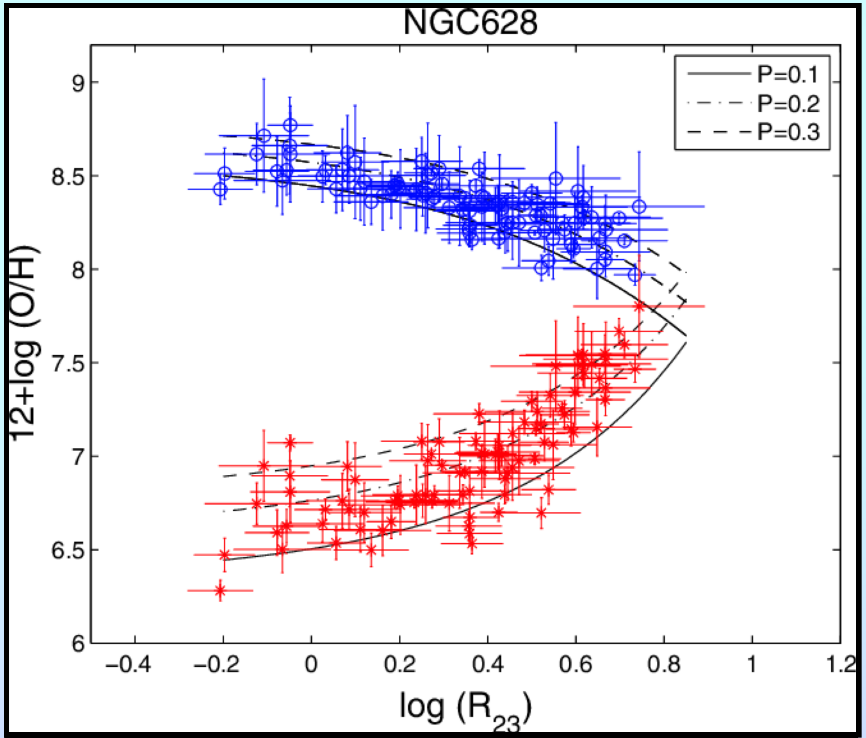
- The 2-2-1 structure of the p^3 configuration is particular sensitive to the density of free electrons. The ratio of [O II] $\lambda3729/\lambda3726$ is best for this, although because the lines are so close together, they are often blended into one "3727" line. [S II] $\lambda6717/\lambda6731$ is just as sensitive, but may be difficult to measure since the abundance of sulfur is generally just ~ 4% that of oxygen.

- Ions with p^2 and p^4 configurations have a 3-1-1 structure, and are useful for measuring the temperature of the free electrons. This is often done with O^{++} via the ratio of $(\lambda5007+\lambda4959)/\lambda4363$. However, the $\lambda4363$ line will generally be 30 to 1200 times weaker than $\lambda5007$, so its detection can be challenging. (N^+ can also be used with $\lambda5755$ as the key line, but often times, most of the nitrogen is doubly, rather than singly ionized.)

Summary of Results

- If one can fix T_e and (to a lesser extent) N_e, then one can determine "direct" ionic abundances from the strengths of the forbidden lines. There is still the issue of how much gas is in the various ionization states, but if one measures abundances for two species (say, O^+ and O^{++}), one can usually solve this problem.

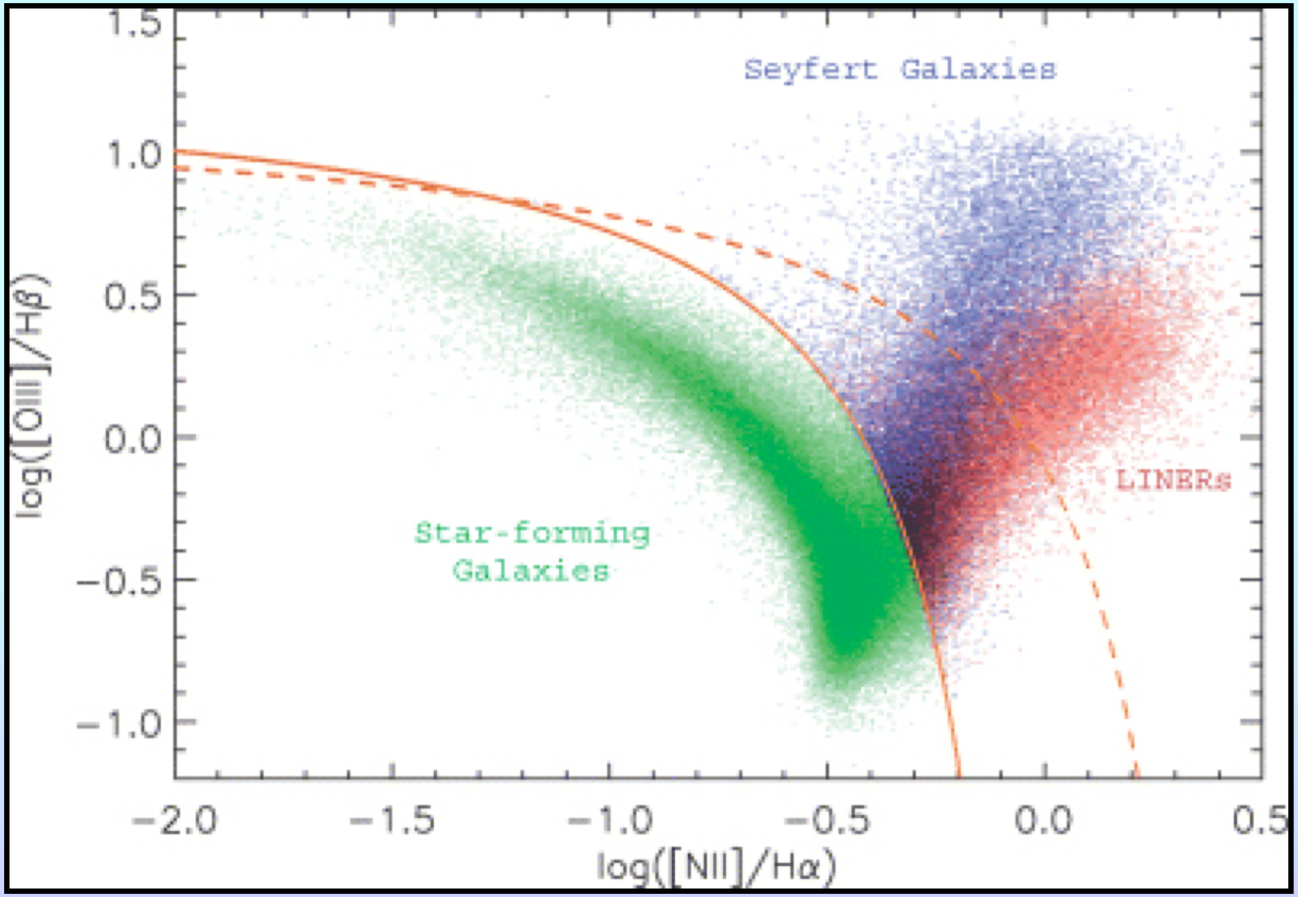
- If one cannot fix T_e and N_e, one can still invoke empirical relationships between line strengths and abundances seen in the local universe. Most extragalactic studies invoke these relationships, but their applicability is not always clear.



R_{23} = ([O III] λ5007 + [O II] λ3727) / Hβ

BPT Diagrams

The ratios of strong emission lines have also been empirically shown to be useful for discriminating star-forming regions and galaxies from active galactic nuclei. The line ratios that do this are conveniently close together in wavelength, and so are unaffected by reddening.



The first people to do this were Balwin, Phillips, & Terlevich (1981), hence the name "BPT" diagram.